Condensed Matter Physic

Crystalline defects

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ELTE

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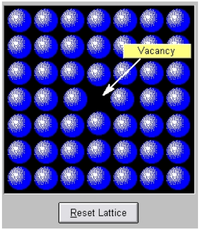
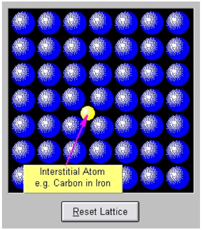
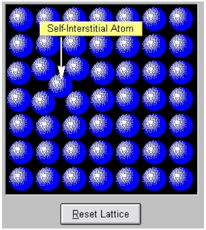
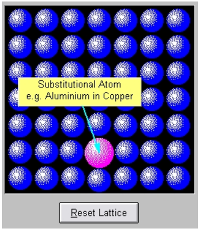
Point defects









Vacancy

Equilibrium vacancy concentration
Gibbs potential

$$G(T,p) = U - TS - pV$$

n vacancy N atom

$$\triangle U = \epsilon_0 n$$

$$\triangle V = v_0 n$$

Entropy

$$S^{config} = k_B \ln \begin{pmatrix} N+n \\ n \end{pmatrix} = k_B \ln \frac{(N+n)!}{N!n!}$$

Stirling-formula

$$\ln n! \approx n \ln n$$

So

$$S^{config} = k_B \left[(N+n)\ln(N+n) - N\ln N - n\ln n \right]$$

From this

$$\triangle G = \epsilon_0 n + p v_0 n - k_B T \left[(N+n)\ln(N+n) - N\ln N - n\ln n \right]$$

Vacancy

Equilibrium concentration

$$\frac{\partial \triangle G}{\partial n} = 0$$

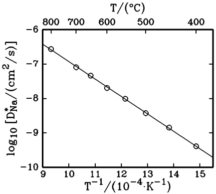
$$\epsilon_0 + pv_0 - k_B T[\ln(N+n) - \ln n] = 0$$

$$\frac{n}{N+n} = e^{-\frac{\epsilon_0 + pv_0}{k_B T}}$$

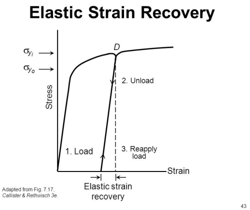
$N >> n$

$$n = Ne^{-\frac{\epsilon_0 + pv_0}{k_B T}}$$

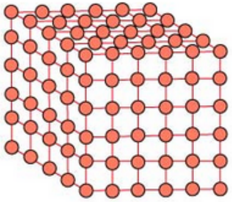
Arrhenius plot (potassium)

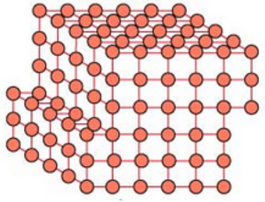


Plastic deformation



Ideal shear





Plastic deformation

Ideal shear

$$F(x) = F_0 \left| \sin\left(\frac{\pi}{a}x\right)\right| = \sigma a^2$$

Small deformation

$$\gamma = \frac{x}{a}, \qquad \sigma = \mu\frac{x}{a}$$

So

$$F_0 = \mu\frac{a^2}{\pi}$$

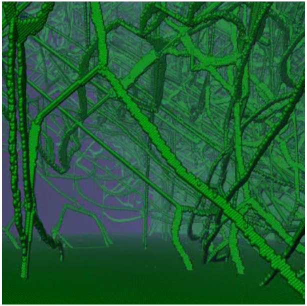
From this

$$\sigma_f \cong \frac{\mu}{\pi} \cong 30 GPa$$

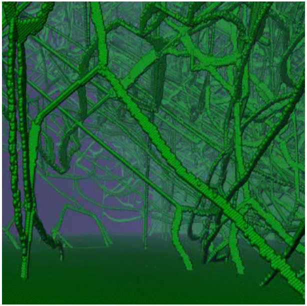
Experiment

$$\sigma_f \cong 100 MPa$$

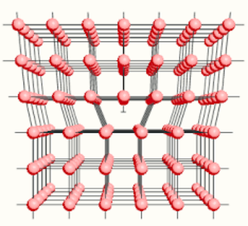
MDD



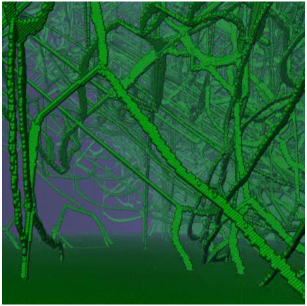
MDD



Polányi, Orován, Taylor (1934)



MDD



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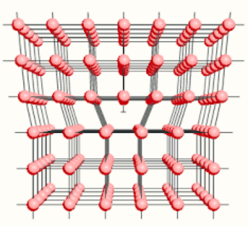
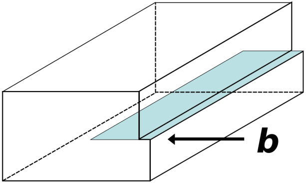


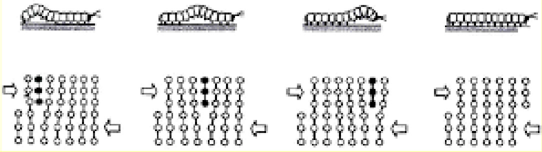
Vito Volterra (1905)



Dislocation

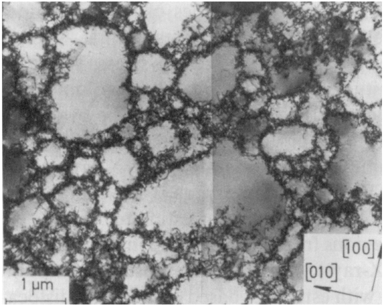
Az elcsúszás nem egyszerre megy végbe

Ez csak akkor lehetséges, ha a kristály tartalmaz egyméretű rácshibákat, diszlokációkat.

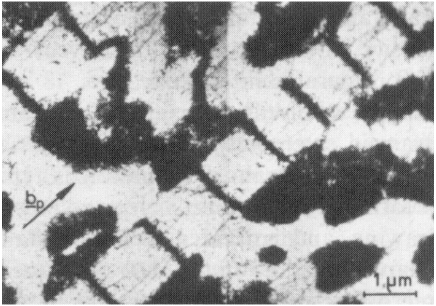


Glide: the number of atom is conserved
Climb: the number of atom is not conserved, requires high temperature.

TEM

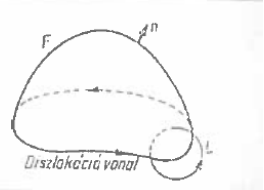


Cell structure



PSB

dislocation density is $\rho = 10^1 4m^{-2}$



Field theory of dislocations

$$\partial_i u_j := \beta_{ij} = \beta^p_{ij} + \beta^e_{ij} \qquad \frac{d\underline{u}}{d\underline{r}} := \hat{\beta} = \hat{\beta}^e + \hat{\beta}^p$$

Dislocation density tensor

$$\alpha_{ij} = e_{ikl}\partial_k \beta^p_{lj} = -e_{ikl}\partial_k \beta^e_{lj} \qquad \hat{\alpha} = \nabla \times \hat{\beta}^p = -\nabla \times \hat{\beta}^e$$

$$b_j = \int_A \alpha_{ij} dA_i$$

$$b_j = -\int_A e_{ikl} \frac{\partial}{\partial r_k} \beta^e_{lj} dA_i = -\oint \beta^e_{ij} ds_i = -\oint du_j.$$

Individual dislocation

$$\alpha_{ij} = l_i b_j \delta(\xi) \qquad (\hat{\alpha} = \underline{l} \circ \underline{b}\delta(\xi))$$

Plastic distortion

$$\beta^p_{ij}(\vec{r}) = n_i b_k \delta(\zeta)$$

Multiple with the elastic constants and take its div:

$$\frac{\partial}{\partial r_i} C_{ijkl} \frac{\partial u_k}{\partial r_l} = \frac{\partial}{\partial r_i} C_{ijkl} \beta^p_{kl} = f_j \left(div\ \hat{C} \frac{d\underline{u}}{d\underline{r}} = div\ \hat{C} \hat{\beta}^p = \underline{f} \right)$$

Displacement field of a screw dislocation

$$u_3 = \frac{b}{2\pi}\varphi$$

Stress field of a straight dislocation $\sigma \propto b/r$

$$\begin{aligned}
\sigma_{11} &= \frac{\mu b}{2\pi(1-\nu)} \frac{y(3x^2+y^2)}{(x^2+y^2)^2} \\
\sigma_{22} &= \frac{\mu b}{2\pi(1-\nu)} \frac{y(x^2-y^2)}{(x^2+y^2)^2} \\
\sigma_{12} &= \frac{\mu b}{2\pi(1-\nu)} \frac{x(x^2-y^2)}{(x^2+y^2)^2}
\end{aligned}$$

Energy of a dislocation

$$\sigma \propto b/r \text{ így } E \propto b^2$$

$$2\left(\frac{b}{2}\right)^2 < b^2$$

$$\underline{b} = \underline{a}_i$$

Fcc $\underline{b} = \frac{1}{2}(1, 1, 0)$
Bcc $\underline{b} = \frac{1}{2}(1, 1, 1)$

Dislocation-dislocation interaction

Elastic energy

$$E = \frac{1}{2}\int \sigma_{ij}\partial_i u_j dV$$

Let us

$$\sigma_{ij} = \sigma_{ij}^{ext} + \sigma_{ij}^{disl}$$
$$u_i = u_i^{ext} + u_i^{disl}$$

leads to

$$E = \frac{1}{2}\int \left[\sigma_{ij}^{ext}\partial_i u_j^{ext} + \sigma_{ij}^{ext}\partial_i u_j^{disl} + \sigma_{ij}^{disl}\partial_i u_j^{ext} + \sigma_{ij}^{disl}\partial_i u_j^{disl}\right] dV$$

Since

$$\sigma_{ij} = C_{ijkl}\partial_i u_j$$

$$E = E_{ext} + E_{disl} + \int \sigma_{ij}^{ext}\partial_i u_j^{disl} dV$$

Dislocation dislocation interaction

$$E_{int} = \int \sigma_{ij}^{ext} \partial_i u_j^{disl} dV$$

Partial integration

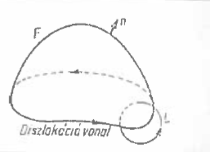
$$E_{int} = \int \partial_i (\sigma_{ij}^{ext} u_j^{disl}) dV - \int (\partial_i \sigma_{ij}^{ext}) u_j^{disl} dV$$

Since

$$\partial_i \sigma_{ij}^{ext} = 0$$

$$E_{int} = \int \partial_i (\sigma_{ij}^{ext} u_j^{disl}) dV = \int (\sigma_{ij}^{ext} u_j^{disl}) dn_i$$

Dislocation-dislocation interaction



$\underline{u}$-nak $\underline{b}$ has a jump on the cut surface!

$$E_{int} = b_j \int_f \sigma_{ij}^{ext} dn_i$$

For the moving line

$$\triangle E_{int} = b_j \oint_v \sigma_{ij}^{ext} (\triangle \underline{r} \times \underline{dl})_i$$

$$\triangle E_{int} = \oint_v (\underline{dl} \times (\hat{\sigma}^{ext} \underline{b}))_i \triangle r_i$$

Peack Koehler force

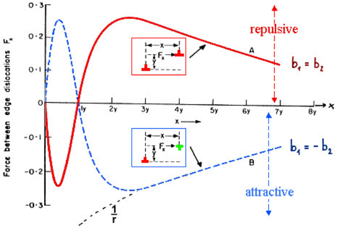
$$\underline{f} = (\hat{\sigma}^{ext} \underline{b}) \times \underline{l}$$

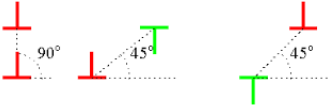
For glide only, we need

$$f_{glide} = [(\hat{\sigma}^{ext}\underline{b}) \times \underline{l}]\frac{\underline{b}}{b} = \underline{n}\hat{\sigma}^{ext}\underline{b} = \tau b \quad \text{ahol} \quad \underline{n} = \frac{\underline{b}}{b} \times \underline{l}$$

Edge dislocation

$$f = b_1 b_2 \frac{\mu}{2\pi(1-\nu)} \frac{x(x^2-d^2)}{(x^2+d^2)^2}$$

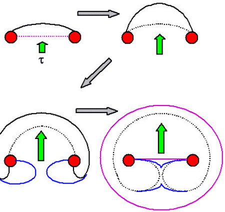




Possible equilibrium configurations

Dislocation multiplication

Frank-Read source

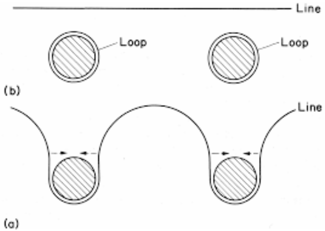


Flow stress (Taylor relation)

$$\tau_f = \alpha \mu b \sqrt{\rho}$$

Work hardening by precipitate

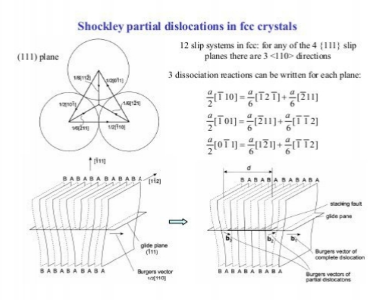
Line tension $\tau_l = E_l/R$

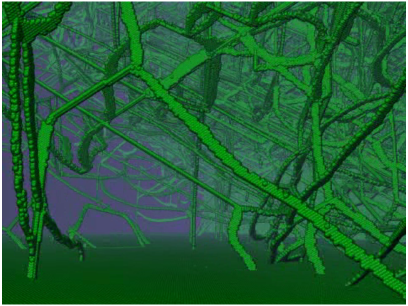


Critical stress

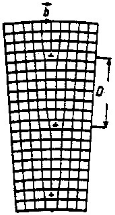
$$\tau_c = \propto \frac{1}{l}$$

Partial dislocation

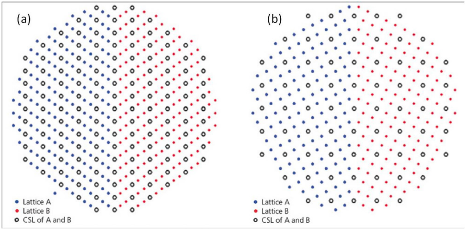




Grain boundary



Small angle grain boundary



Coincidence lattice (Σn)